

VALERIC ANHYDRIDE

Other names:	Pentanoic acid, anhydride n-Valeric anhydride pentanoic anhydride
Inchi:	InChI=1S/C10H18O3/c1-3-5-7-9(11)13-10(12)8-6-4-2/h3-8H2,1-2H3
InchiKey:	DUCKXCGALKOSJF-UHFFFAOYSA-N
Formula:	C10H18O3
SMILES:	CCCCC(=O)OC(=O)CCCC
Mol. weight [g/mol]:	186.25

Physical Properties

Property code	Value	Unit	Source
af	0.6779		Cheméo Relay (1.0)
gf	-329.52	kJ/mol	Joback Method
hf	-749.41	kJ/mol	Cheméo Relay (1.0)
hfus	26.04	kJ/mol	Joback Method
hvap	54.90	kJ/mol	Cheméo Relay (1.0)
ie	10.03	eV	Cheméo Relay (1.0)
log10ws	-2.76		Cheméo Relay (1.0)
logp	2.437		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	1283.10		NIST Webbook
rinpol	1283.10		NIST Webbook
tb	459.50 ± 0.30	K	NIST Webbook
tc	662.65	K	Cheméo Relay (1.0)
tf	217.05 ± 0.70	K	NIST Webbook
vc	0.620	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.21	J/mol×K	558.36	Joback Method
cpg	403.56	J/mol×K	588.52	Joback Method
cpg	416.35	J/mol×K	618.67	Joback Method

cpg	428.57	J/mol×K	648.83	Joback Method
cpg	440.25	J/mol×K	678.99	Joback Method
cpg	451.38	J/mol×K	709.15	Joback Method
cpg	461.96	J/mol×K	739.30	Joback Method
dvisc	0.0026272	Pa×s	324.55	Joback Method
dvisc	0.0014182	Pa×s	363.52	Joback Method
dvisc	0.0008627	Pa×s	402.49	Joback Method
dvisc	0.0005729	Pa×s	441.45	Joback Method
dvisc	0.0004066	Pa×s	480.42	Joback Method
dvisc	0.0003038	Pa×s	519.39	Joback Method
dvisc	0.0002364	Pa×s	558.36	Joback Method
rho	939.15	kg/m ³	298.15	Excess Molar Enthalpies of Binary Systems of n-Valeric Anhydride or n-Hexanoic Anhydride with n-Dodecane, n-Tetradecane, or n-Hexadecane at 298.15 K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.70	K	2.10	NIST Webbook
tbrp	384.20	K	2.00	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2082599&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Excess Molar Enthalpies of Binary Systems of n-Valeric Anhydride or n-Hexanoic Anhydride with n-Dodecane, n-Tetradecane, or n-Hexadecane at 298.15 K: <https://www.doi.org/10.1021/je900598y>

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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